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QUADRATURE OVER THE SPHERE *

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Abstract. Consider integration over the unit sphere in $\mathbb{R}^3$, especially when the integrand has singular behaviour in a polar region. In an earlier paper [4], a numerical integration method was proposed that uses a transformation that leads to an integration problem over the unit sphere with an integrand that is much smoother in the polar regions of the sphere. The transformation uses a *grading parameter* q. The trapezoidal rule is applied to the spherical coordinates representation of the transformed problem. The method is simple to apply, and it was shown in [4] to have convergence $O\left(h^{2q}\right)$ or better for integer values of $2q$. In this paper, we extend those results to non-integral values of $2q$. We also examine superconvergence that was observed when $2q$ is an odd integer. The overall results agree with those of [11], although the latter is for a different, but related, class of transformations.

Key words. spherical integration, trapezoidal rule, Euler-MacLaurin expansion

AMS subject classifications. 65D32

1. Introduction. In the earlier paper [4] a quadrature method for the sphere was introduced to deal with an integrand that is singular at either the north or south pole of the sphere. The present paper addresses some of the conjectures that were left unanswered in that earlier paper.

The earlier paper studied the more general problem of quadrature over a smooth surface S,

$$I(F) = \int_S F(Q)\, dS_Q \tag{1.1}$$

in which S is the image of a smooth mapping defined on the unit sphere $U \subseteq \mathbb{R}^3$,

$$\mathcal{M} : U \xrightarrow[onto]{1-1} S \tag{1.2}$$

Using this mapping the quadrature problem reduces to that of integration over U,

$$I(f) = \int_U f(Q)\, dS_Q \tag{1.3}$$

and that is the case we address here. We assume f is several times continuously differentiable over the unit sphere U, with the precise order of differentiability to be specified later. In the following section we define the numerical method and we give the main results of the paper. Subsequent sections deal with the proofs of those results.

This problem has also been studied by A. Sidi [11], and some of our tools are closely related to those used in his paper. In [11] Sidi develops a class of single variable transformations to improve the behaviour of the integrand in (1.3). This class is denoted as the "extended class $\mathcal{S}_m$", or "class $\mathcal{S}_m$" for short, and it is an extension of that developed earlier in [9]. A particular member of this class that is studied in [11] is the $\sin^m$-transformation, and the numerical examples there are done with this transformation. Some of the tools used in Sidi's paper [11] are similar to ones we use, although there are differences as well because our transformation does not belong to the class he addresses. The overall asymptotic error results

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that we give are, in the end, the same as his, even though the underlying transformations are different. Our results are not as complete as those of Sidi, due in part to the lack of needed mathematical tools as compared to those developed in [11] for the class $\mathcal{S}_m$ transformations analyzed there.

2. The numerical method. In spherical coordinates this integral (1.3) can be written as

$$I(f) = \int_0^{\pi} \int_0^{2\pi} f\left(\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta\right) \sin\theta \, d\phi \, d\theta$$

Rather than approximating this integral directly, we begin by introducing a transformation $\mathcal{L} : U \xrightarrow[onto]{1-1} U$. With respect to spherical coordinates on U,

(2.1)
$$\mathcal{L} : Q = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta) \mapsto \widetilde{Q} = \frac{(\cos\phi\sin^q\theta, \sin\phi\sin^q\theta, \cos\theta)}{\sqrt{\cos^2\theta + \sin^{2q}\theta}} \equiv L(\phi,\theta)$$

In this transformation, $q \geq 1$ is a 'grading parameter'. The north and south poles of U remain fixed, while the region around them is distorted by the mapping.

The integral $I(f)$ becomes

$$I(f) = \int_U f\left(\mathcal{L}(\widetilde{Q})\right) J_{\mathcal{L}}\left(\widetilde{Q}\right) dS_{\widetilde{Q}} \tag{2.2}$$

with $J_{\mathcal{L}}\left(\widetilde{Q}\right)$ the Jacobian of the mapping $\mathcal{L}$,

$$J_{\mathcal{L}}\left(\widetilde{Q}\right) = |D_\phi L(\phi,\theta) \times D_\theta L(\phi,\theta)| = \frac{\sin^{2q-1}\theta\left(q\cos^2\theta + \sin^2\theta\right)}{\left(\sin^{2q}\theta + \cos^2\theta\right)^{\frac{3}{2}}} \tag{2.3}$$

In spherical coordinates,

$$\begin{aligned} I(f) &= \int_0^{\pi} \frac{\sin^{2q-1}\theta\left(q\cos^2\theta + \sin^2\theta\right)}{\left(\sin^{2q}\theta + \cos^2\theta\right)^{\frac{3}{2}}} \int_0^{2\pi} f\left(\xi,\eta,\zeta\right) \, d\phi \, d\theta \\ (\xi,\eta,\zeta) &= \frac{(\cos\phi\sin^q\theta, \sin\phi\sin^q\theta, \cos\theta)}{\sqrt{\sin^{2q}\theta + \cos^2\theta}} \end{aligned} \tag{2.4}$$

For $n \geq 1$, let $h = \pi/n$, and

$$\phi_j = \theta_j = jh$$

For a generic function g, introduce the bivariate trapezoidal approximation

$$\int_0^{\pi} \int_0^{2\pi} g(\sin\theta, \cos\theta, \sin\phi, \cos\phi) \, d\phi \, d\theta \approx h^2 \sum_{k=0}^{n}{}'' \sum_{j=0}^{2n}{}'' g(\sin\theta_k, \cos\theta_k, \sin\phi_j, \cos\phi_j)$$

in which the superscript notation $''$ means to multiply the first and last terms by $\frac{1}{2}$ before summing. Apply this to (2.4). Note that the integrand is zero for $\theta = 0, \pi$ and that the

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integrand has period 2π in ϕ. Therefore

$$\int_0^\pi \int_0^{2\pi} g(\sin\theta, \cos\theta, \sin\phi, \cos\phi)\, d\phi\, d\theta$$

$$\approx h^2 \sum_{k=1}^{n-1} \sum_{j=1}^{2n} g(\sin\theta_k, \cos\theta_k, \sin\phi_j, \cos\phi_j) \equiv \mathcal{T}_n \tag{2.5}$$

$$g(\sin\theta, \cos\theta, \sin\phi, \cos\phi) = \frac{\sin^{2q-1}\theta \left(q\cos^2\theta + \sin^2\theta\right)}{\left(\sin^{2q}\theta + \cos^2\theta\right)^{\frac{3}{2}}} f(\xi, \eta, \zeta)$$

with (ξ, η, ζ) as in (2.4).

When $2q$ is an integer, we were able in [4] to show an accelerated rate of convergence for this numerical integration of (1.3), as follows.

THEOREM 2.1. *For the grading parameter q in the integral (2.4), assume $q \geq 1$ and $2q$ is a positive integer. Introduce*

$$p = \begin{cases} 2q, & 2q \text{ even} \\ 2q+1, & 2q \text{ odd} \end{cases}$$

Assume f is p-times differentiable with $f^{(p)} \in L^1(U)$, the space of Lebesgue integrable functions on U. Then the error in approximating (1.3) by (2.5) satisfies

$$I - \mathcal{T}_n = O\left(h^p\right) \tag{2.6}$$

We left some questions unanswered in the earlier paper and two of those are addressed in this paper.

- First, what happens when $2q$ is not an integer.
- Second, when $2q$ is an odd integer, what is the actual rate of convergence? We observed in [4] a much faster rate of convergence in such a case.

The most important tool used in understanding both of these questions is the Euler-MacLaurin expansion (e.g. see [3, p. 285], [10, Appendix D]) and its generalization in Lyness and Ninham [6]. A modification of the latter is used in answering the first question given above, and the regular Euler-MacLaurin expansion is used in exploring the second question. We present theorems that generalize the above Theorem 2.1, demonstrating them in later sections.

THEOREM 2.2. *Assume the grading parameter q satisfies $1 < q < 2$, $q \neq 1.5$. Let $p = 1 + [2q]$, with $[2q]$ denoting the integer part of $2q$. Assume f is p-times differentiable with all p^{th}-derivatives of f belonging to $L^1(U)$. Then*

$$I - \mathcal{T}_n = O\left(h^{2q}\right) \tag{2.7}$$

After giving a proof in Section 3, we indicate how the theorem may be extended to other larger non-integral values of $2q$. We further note that this theorem corresponds to Theorem 4.3 in [11], although the latter is for a different class of transformations.

THEOREM 2.3. *Assume $q = 1.5$ or $q = 2.5$ or $q = 3.5$ and let $p = 4q$. Assume f is p-times differentiable with all p^{th}-order derivatives of f belonging to $L^1(U)$. Then*

$$I - \mathcal{T}_n = O\left(h^{4q}\right) \tag{2.8}$$

Again, following the proof in Section 4, we indicate how the theorem can be extended to other cases in which $2q$ is an odd integer. This theorem also agrees with Theorem 4.3 in [11] for the transformations covered there.

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We remark on the differentiability assumptions about f over U. Suppose f is a function defined on only U, and suppose all derivatives of f of order $\leq p$, with respect to local coordinate systems on U, are continuous. Then it is known that f can be extended to some ε-neighborhood of U with preservation of the differentiability. In the following theory, without loss of generality, we assume that the integrand f is defined on an ε-neighborhood of U for some $\varepsilon > 0$. Thus we treat $f(\xi, \eta, \zeta)$ as a differentiable function of three variables, not two.

As in [4], we decompose the calculation of the error $I - \mathcal{T}_n$ into two portions:

$$\begin{aligned} I(f) - \mathcal{T}_n = & \int_0^\pi \frac{\sin^{2q-1}\theta\left(q\cos^2\theta + \sin^2\theta\right)}{\left(\sin^{2q}\theta + \cos^2\theta\right)^{\frac{3}{2}}} \int_0^{2\pi} f(\xi, \eta, \zeta)\, d\phi\, d\theta \\ & -h\sum_{k=1}^{n-1} \frac{\sin^{2q-1}\theta_k\left(q\cos^2\theta_k + \sin^2\theta_k\right)}{\left(\sin^{2q}\theta_k + \cos^2\theta_k\right)^{\frac{3}{2}}} \int_0^{2\pi} f(\xi_k, \eta_k, \zeta_k)\, d\phi \\ & +h\sum_{k=1}^{n-1} \frac{\sin^{2q-1}\theta_k\left(q\cos^2\theta_k + \sin^2\theta_k\right)}{\left(\sin^{2q}\theta_k + \cos^2\theta_k\right)^{\frac{3}{2}}} \\ & \times \left[\int_0^{2\pi} f(\xi_k, \eta_k, \zeta_k)\, d\phi - h\sum_{j=1}^{2n} f(\xi_{k,j}, \eta_{k,j}, \zeta_{k,j})\right] \end{aligned} \tag{2.9}$$

The last portion is the trapezoidal error for a periodic integral over $[0, 2\pi]$, and it is straightforward to deal with if f is assumed sufficiently differentiable, obtaining the correct order of convergence for $I - \mathcal{T}_n$. More precisely, with respect to the integration variable ϕ, the integrand is a smooth differentiable periodic function over $[0, 2\pi]$. In the remainder of this paper, we consider only the first portion of the error, that of the trapezoidal rule applied over $0 \leq \theta \leq \pi$.

3. Convergence with $2q$ non-integral. The key tool we use is a modification of a result of Lyness and Ninham [6]. The proof of the modification (Lyness [7]) is based on recent techniques developed in Monegato and Lyness [8]. We use mostly the notation of [6], specializing the results in it to our situation. Consider approximating the integral

$$I = \int_0^1 D(\tau)\, d\tau$$

with $D(\tau)$ having the form

$$D(\tau) = \tau^\lambda (1-\tau)^\omega h(\tau) \tag{3.1}$$

$$= \tau^\lambda \psi_0(\tau) = (1-\tau)^\omega \psi_1(\tau) \tag{3.2}$$

with $0 < \lambda, \omega < 1$. We assume $h(\tau)$ is N-times continuously differentiable on $[0, 1]$ for some $N \geq 1$. Consider the error in the trapezoidal rule applied to I,

$$E_m = \frac{1}{m}\sum_{j=0}^{m}{}'' D\left(\frac{j}{m}\right) - \int_0^1 D(\tau)\, d\tau \tag{3.3}$$

Then

$$\begin{aligned} E_m = & \sum_{s=0}^{N} \frac{\psi_0^{(s)}(0)}{s!} \cdot \frac{\zeta(-\lambda - s)}{m^{\lambda+s+1}} \\ & + \sum_{s=0}^{N} \frac{(-1)^s\, \psi_1^{(s)}(1)}{s!} \cdot \frac{\zeta(-\omega - s)}{m^{\omega+s+1}} + o\left(m^{-(\lambda+N+1)}\right) + o\left(m^{-(\omega+N+1)}\right) \end{aligned} \tag{3.4}$$

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In this we use the Riemann zeta function $\zeta(s)$.

From (2.4), the integrand for our application of (3.4) is the function

$$D(\tau) = (\sin(\tau\pi))^{2q-1} \beta\left(\sin^2(\tau\pi)\right) \int_0^{2\pi} f(\xi, \eta, \zeta)\, d\phi, \qquad 0 \le \tau \le 1 \tag{3.5}$$

where

$$\beta(t) = \frac{(1-q)\,t + q}{(t^q - t + 1)^{\frac{3}{2}}}$$

$$(\xi, \eta, \zeta) = \frac{(\cos\phi \sin^q(\tau\pi), \sin\phi \sin^q(\tau\pi), \cos(\tau\pi))}{\sqrt{\sin^{2q}(\tau\pi) + \cos^2(\tau\pi)}}$$

and with f assumed sufficiently smooth on an open neighborhood of the unit sphere.

Let δ be the fractional part of $2q$,

$$\delta = 2q - [2q], \qquad 0 < \delta < 1$$

Rewrite our integrand as

$$\begin{aligned} D(\tau) &= \tau^\delta (1-\tau)^\delta \left(\frac{\sin(\tau\pi)}{\tau(1-\tau)}\right)^\delta (\sin(\tau\pi))^{2q-\delta-1} \beta\left(\sin^2(\tau\pi)\right) \int_0^{2\pi} f(\xi, \eta, \zeta)\, d\phi \\ &= \tau^\delta \psi_0(\tau) = (1-\tau)^\delta \psi_1(\tau) \end{aligned}$$

We must show that the function $\psi_0(\tau)$ is p-times differentiable with $\psi_0(\tau)$ locally integrable about $\tau = 0$; and similarly with respect to $\psi_1(\tau)$ about $\tau = 1$. We treat separately the cases of $1 < q < 1.5$ and $1.5 < q < 2$.

3.1. Case 1: $1 < q < 1.5$**.** We have $[2q] = 2$ and $2q = 2 + \delta$; and then

$$\begin{aligned} D(\tau) &= \tau^\delta (1-\tau)^\delta \left(\frac{\sin(\tau\pi)}{\tau(1-\tau)}\right)^\delta \sin(\tau\pi)\, \beta\left(\sin^2(\tau\pi)\right) \int_0^{2\pi} f(\xi, \eta, \zeta)\, d\phi \\ &= \tau^\delta \psi_0(\tau) = (1-\tau)^\delta \psi_1(\tau) \end{aligned}$$

where

$$\psi_0(\tau) = (1-\tau)^\delta \left(\frac{\sin(\tau\pi)}{\tau(1-\tau)}\right)^\delta \sin(\tau\pi)\, \beta\left(\sin^2(\tau\pi)\right) \int_0^{2\pi} f(\xi, \eta, \zeta)\, d\phi$$

and similarly so for $\psi_1(\tau)$. Note that

$$\frac{\sin(\tau\pi)}{\tau(1-\tau)} \ge \pi, \qquad 0 \le \tau \le 1$$

and then easily

$$\left(\frac{\sin(\tau\pi)}{\tau(1-\tau)}\right)^\delta$$

is analytic on $[0, 1]$.

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To obtain an error of size $O\left(m^{-2q}\right)$, as asserted in (2.7), we must take $N = 3$ in (3.4). The error formula becomes

$$E = \sum_{s=0}^{2} \frac{\psi_0^{(s)}(0)}{s!} \frac{\zeta(-\delta - s)}{m^{\delta+s+1}} \tag{3.6}$$
$$+ \sum_{s=0}^{2} \frac{(-1)^s \psi_1^{(s)}(1)}{s!} \frac{\zeta(-\delta - s)}{m^{\delta+s+1}} + O\left(m^{-3}\right)$$

Using this to show $E = O\left(m^{-2q}\right)$ requires:

1. $\psi_0(0) = 0, \psi_1(1) = 0$;
2. $\psi_0, \psi_1 \in C^2$ in neighborhoods of $\tau = 0$ and $\tau = 1$, respectively, and $\psi_0^{(j)}(0) = \psi_1^{(j)}(1) = 0$ for $j = 1, 2$;
3. $\psi_0^{(3)}, \psi_1^{(3)} \in L^1$ in neighborhoods of $\tau = 0$ and $\tau = 1$, respectively.

The first condition is immediate.

We give arguments for only $\psi_0(t)$, but analogous arguments hold for $\psi_1(t)$. To find the derivatives of $\psi_0(\tau)$, we must differentiate the product

$$(1-\tau)^\delta \left(\frac{\sin(\tau\pi)}{\tau(1-\tau)}\right)^\delta \sin(\tau\pi)\, h(\tau) H(\tau) \tag{3.7}$$

where

$$h(\tau) = \beta\left(\sin^2(\tau\pi)\right) \tag{3.8}$$
$$H(\tau) = \int_0^{2\pi} f(\xi, \eta, \zeta)\, d\phi$$

We need to consider the behaviour of the derivatives around the endpoints of $[0, 1]$. Since the first two terms in (3.7),

$$(1-\tau)^\delta \left(\frac{\sin(\tau\pi)}{\tau(1-\tau)}\right)^\delta$$

are analytic in a neighborhood of $\tau = 0$, we need consider only the derivatives of the product

$$\sin(\tau\pi)\, h(\tau) H(\tau) \tag{3.9}$$

Recall

$$\beta(t) = \frac{(1-q)\,t + q}{(t^q - t + 1)^{\frac{3}{2}}}$$

We need the derivatives of

$$h(\tau) = \beta\left(\sin^2(\tau\pi)\right) = \beta\left(\tfrac{1}{2}\left[1 - \cos(2\tau\pi)\right]\right)$$

Use the following to do so.

$$h(\tau) = \beta(g(\tau)), \qquad g(\tau) = \tfrac{1}{2}\left[1 - \cos(2\tau\pi)\right]$$
$$h'(\tau) = \beta'(g(\tau))\, g'(\tau)$$
$$h^{(2)}(\tau) = \beta^{(2)}(g(\tau))\,(g'(\tau))^2 + \beta'(g(\tau))\, g^{(2)}(\tau) \tag{3.10}$$
$$h^{(3)}(\tau) = \beta^{(3)} \cdot (g')^3 + 3\beta^{(2)} \cdot g' \cdot g^{(2)} + \beta' \cdot g^{(3)}$$
$$h^{(4)}(\tau) = \beta^{(4)} \cdot (g')^4 + 6\beta^{(3)} \cdot (g')^2 \cdot g^{(2)}$$
$$+ 3\beta^{(2)} \cdot \left(g^{(2)}\right)^2 + 4\beta^{(2)} \cdot g' \cdot g^{(3)} + \beta' \cdot g^{(4)}$$

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These are special cases of the Faa di Bruno [15] formula for the n^{th} derivative of a composite function:

$$
\begin{aligned}
D^n\beta\left(g(\tau)\right) = \sum_k \frac{n!}{k_1!\cdots k_n!}\left(D^{|k|}\beta\right)\left(g(\tau)\right) \\
\times\left(\frac{Dg(\tau)}{1!}\right)^{k_1}\left(\frac{D^2g(\tau)}{2!}\right)^{k_2}\cdots\left(\frac{D^ng(\tau)}{n!}\right)^{k_n}
\end{aligned}
\tag{3.11}
$$

with k a multi-integer satisfying

$$
\begin{aligned}
&k = (k_1,\dots,k_n), \quad \text{all } k_j \geq 0\\
&|k| = k_1+\cdots+k_n\\
&k_1+2k_2+\cdots+nk_n = n
\end{aligned}
$$

Next, in general for an integer $\ell > 0$,

$$
g^{(\ell)}(\tau) = \begin{cases} \pm\frac{1}{2}(2\pi)^\ell\sin(2\pi\tau), & \ell \text{ odd}\\ \pm\frac{1}{2}(2\pi)^\ell\cos(2\pi\tau), & \ell \text{ even}\end{cases}
$$

For the function $\beta(t)$,

$$
\begin{aligned}
\beta'(t) &= \frac{c_1t^{q-1} + \textit{terms that are smoother than } t^{q-1}}{(t^q-t+1)^{\frac{5}{2}}}\\
\beta^{(2)}(t) &= \frac{c_2t^{q-2} + \textit{terms that are smoother than } t^{q-2}}{(t^q-t+1)^{\frac{7}{2}}}
\end{aligned}
$$

Since $q = 1+\frac{1}{2}\delta$ for the current case, we have that $\beta^{(2)}(t)$ is singular at $t=0$. For a general q not an integer,

$$
\beta^{(k)}(t) = \frac{c_kt^{q-k} + \textit{terms that are smoother than } t^{q-k}}{(t^q-t+1)^{(2k+3)/2}}, \qquad k\geq 1
\tag{3.12}
$$

Combining these results for derivatives of g and β, we have

$$
\begin{aligned}
h'(\tau) &= O\left((\sin(\pi\tau))^{2(q-1)+1}\right) = O\left((\sin(\pi\tau))^{2q-1}\right)\\
&= O\left((\sin(\pi\tau))^{1+\delta}\right)\\
h^{(2)}(\tau) &= O\left((\sin(\pi\tau))^{\min[2(q-2)+2,\ 2(q-1)]}\right) = O\left((\sin(\pi\tau))^{2q-2}\right)\\
&= O\left((\sin(\pi\tau))^{\delta}\right)\\
h^{(3)}(\tau) &= O\left((\sin(\pi\tau))^{\min[2(q-3)+3,\ 2(q-2)+1, 2(q-1)+1]}\right) = O\left((\sin(\pi\tau))^{2q-3}\right)\\
&= O\left((\sin(\pi\tau))^{-1+\delta}\right)
\end{aligned}
\tag{3.13}
$$

Note that $-1 < -1+\delta < 0$. Thus $h^{(3)}(\tau)$ is integrable over $[0,1]$. Also, $h^{(2)}(\tau)$ is continuous on $[0,1]$ with $h^{(2)}(0) = h^{(2)}(1) = 0$.

What are the derivatives of

$$
H(\tau) = \int_0^{2\pi} f(\xi,\eta,\zeta)\ d\phi
$$

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where

$$
\begin{aligned}
(\xi, \eta, \zeta) &= \frac{\left(\cos\phi \sin^q(\tau\pi), \sin\phi \sin^q(\tau\pi), \cos(\tau\pi)\right)}{\sqrt{R(\tau)}} \\
&= \frac{\left(\cos\phi \sin^{1+\delta/2}(\tau\pi), \sin\phi \sin^{1+\delta/2}(\tau\pi), \cos(\tau\pi)\right)}{\sqrt{R(\tau)}} \\
R(\tau) &= \sin^{2q}(\tau\pi) + \cos^2(\tau\pi) = \sin^{2+\delta}(\tau\pi) + \cos^2(\tau\pi)
\end{aligned}
$$

By the chain rule,

$$H'(\tau) = \int_0^{2\pi} \left[f_1 \frac{d\xi}{d\tau} + f_2 \frac{d\eta}{d\tau} + f_3 \frac{d\zeta}{d\tau} \right] d\phi$$

To obtain the behaviour as a function of τ, we use

$$
\begin{aligned}
\begin{bmatrix} \dfrac{d\xi}{d\tau} \\ \dfrac{d\eta}{d\tau} \end{bmatrix} &= \pi \sin^{q-1}(\tau\pi) \left[\frac{q\cos(\tau\pi)}{\sqrt{R(\tau)}} \right. \\
&\qquad \left. - \frac{\sin(\tau\pi)\sin(2\tau\pi)\left[q\sin^{2q-2}(\tau\pi) - 1\right]}{2R(\tau)\sqrt{R(\tau)}} \right] \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix} \\
\frac{d\zeta}{d\tau} &= -\pi\sin(\tau\pi) \left[\frac{1}{\sqrt{R(\tau)}} + \frac{\cos^2(\tau\pi)\left[q\sin^{2q-2}(\tau\pi) - 1\right]}{R(\tau)\sqrt{R(\tau)}} \right]
\end{aligned}
$$

For our case of $2q = 2 + \delta$,

$$
\begin{aligned}
\begin{bmatrix} \dfrac{d\xi}{d\tau} \\ \dfrac{d\eta}{d\tau} \end{bmatrix} &= \pi \sin^{\delta/2}(\tau\pi) \left[\frac{q\cos(\tau\pi)}{\sqrt{R(\tau)}} - \frac{\sin(\tau\pi)\sin(2\tau\pi)\left[q\sin^{\delta}(\tau\pi) - 1\right]}{2R(\tau)\sqrt{R(\tau)}} \right] \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix} \\
&= O\left(\sin^{\delta/2}(\tau\pi)\right) \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix} \\
\frac{d\zeta}{d\tau} &= -\pi\sin(\tau\pi) \left[\frac{1}{\sqrt{R(\tau)}} + \frac{\cos^2(\tau\pi)\left[q\sin^{\delta}(\tau\pi) - 1\right]}{R(\tau)\sqrt{R(\tau)}} \right] \\
&= O\left(\sin(\tau\pi)\right)
\end{aligned}
$$

For the second derivative,

$$
\begin{aligned}
H^{(2)}(\tau) = \int_0^{2\pi} &\left[f_{1,1}\left(\frac{d\xi}{d\tau}\right)^2 + f_{2,2}\left(\frac{d\eta}{d\tau}\right)^2 + f_{3,3}\left(\frac{d\zeta}{d\tau}\right)^2 \right. \\
&+ 2f_{1,2}\frac{d\xi}{d\tau}\frac{d\eta}{d\tau} + 2f_{1,3}\frac{d\xi}{d\tau}\frac{d\zeta}{d\tau} + 2f_{2,3}\frac{d\eta}{d\tau}\frac{d\zeta}{d\tau} \\
&\left. + f_1\frac{d^2\xi}{d\tau^2} + f_2\frac{d^2\eta}{d\tau^2} + f_3\frac{d^2\zeta}{d\tau^2} \right] d\phi
\end{aligned}
$$

For the present case that $1 < q < 1.5$, we can continue with this to show that

$$H^{(\ell)}(\tau) = O\left([\sin(\tau\pi)]^{\min[\delta/2 - \ell + 1, 0]} \right), \qquad \ell = 0, 1, 2, 3 \tag{3.14}$$

to show the singular nature of $H^{(2)}$ and $H^{(3)}$.

Now to (3.7), we calculate the derivatives of the product

$$\sin\left(\tau\pi\right)h(\tau)H(\tau)$$

Using Leibniz's formula,

$$\frac{d^{\ell}}{d\tau^{\ell}}\left[\sin\left(\tau\pi\right)h(\tau)H(\tau)\right]=\sum_{|\alpha|=\ell}\frac{\ell!}{\alpha_1!\alpha_2!\alpha_3!}\frac{d^{\alpha_1}}{d\tau^{\alpha_1}}\left[\sin\left(\tau\pi\right)\right]\frac{d^{\alpha_2}}{d\tau^{\alpha_2}}\left[h(\tau)\right]\frac{d^{\alpha_3}}{d\tau^{\alpha_3}}\left[H(\tau)\right] \tag{3.15}$$

where $\alpha=(\alpha_1,\alpha_2,\alpha_3)$, $\alpha_j\geq 0$. There are $\frac{1}{2}\left(\ell+1\right)\left(\ell+2\right)$ terms in this expansion. Consider $\ell=2,3$.

- $\ell=2$. The corresponding values of α are

$$(2,0,0)\,,(1,1,0)\,,(1,0,1)\,,(0,2,0)\,,(0,1,1)\,,(0,0,2)$$

- $\ell=3$. The corresponding values of α are

$$\begin{aligned}&(3,0,0)\,,(2,1,0)\,,(2,0,1)\,,(1,2,0)\,,(1,1,1)\,,\\&(1,0,2)\,,(0,3,0)\,,(0,2,1)\,,(0,1,2)\,,(0,0,3)\end{aligned} \tag{3.16}$$

It is easily checked that all product terms in (3.15) with $\ell=2$ are continuous, even though $H^{(2)}(\tau)$ is singular.

For $\ell=3$, we need to look only at terms containing $h^{(3)}(\tau)$ $[\alpha=(0,3,0)]$ or $H^{(k)}(\tau)$, $k=2,3$ $[\alpha=(1,0,2)\,,(0,1,2),(0,0,3)]$, in order to check for integrability. It is easily checked that in these cases the corresponding terms in (3.15) are integrable. Thus $\psi_0^{(3)}\in L^1$ in a neighborhood of $\tau=0$. An exactly analogous proof works in examing the behaviour of $\psi_1(\tau)$ about $\tau=1$. This completes the proof of $E=O\left(m^{-2q}\right)$ for the case of $1<q<1.5$.

3.2. Case 2: $1.5<q<2$. We have $[2q]=3$ and $2q=3+\delta$; and then

$$\begin{aligned}D(\tau)&=\tau^{\delta}\left(1-\tau\right)^{\delta}\left(\frac{\sin\left(\tau\pi\right)}{\tau\left(1-\tau\right)}\right)^{\delta}\sin^2\left(\tau\pi\right)\beta\left(\sin^2\left(\tau\pi\right)\right)\int_0^{2\pi}f\left(\xi,\eta,\zeta\right)\,d\phi\\&=\tau^{\delta}\psi_0(\tau)=\left(1-\tau\right)^{\delta}\psi_1(\tau)\end{aligned}$$

$$\psi_0(\tau)=\left(1-\tau\right)^{\delta}\left(\frac{\sin\left(\tau\pi\right)}{\tau\left(1-\tau\right)}\right)^{\delta}\sin^2\left(\tau\pi\right)\beta\left(\sin^2\left(\tau\pi\right)\right)\int_0^{2\pi}f\left(\xi,\eta,\zeta\right)\,d\phi$$

and similarly for $\psi_1(\tau)$.

To obtain an error of size $O\left(m^{-2q}\right)$, we must take $N=4$ in (3.4). The error formula becomes

$$\begin{aligned}E=&\sum_{s=0}^{3}\frac{\psi_0^{(s)}(0)}{s!}\frac{\zeta\left(-\delta-s\right)}{m^{\delta+s+1}}\\&+\sum_{s=0}^{3}\frac{\left(-1\right)^s\psi_1^{(s)}(1)}{s!}\frac{\zeta\left(-\delta-s\right)}{m^{\delta+s+1}}+O\left(m^{-4}\right)\end{aligned} \tag{3.17}$$

Using this to show $E=O\left(m^{-2q}\right)$ requires:

1. $\psi_0(0)=\psi_0'(0)=0$, $\psi_1(1)=\psi_1'(1)=0$;

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2. $\psi_0, \psi_1 \in C^3$ in neighborhoods of $\tau = 0$ and $\tau = 1$, respectively;
3. $\psi_0^{(4)}, \psi_1^{(4)} \in L^1$ in neighborhoods of $\tau = 0$ and $\tau = 1$, respectively.

Again, the first condition is straightforward, because of the presence of $\sin^2(\tau\pi)$ in the formulas for $\psi_0(\tau)$ and $\psi_1(\tau)$.

In analogy with the first case, we must consider the derivatives of

$$\sin^2(\tau\pi)\, h(\tau) H(\tau) \tag{3.18}$$

Note that it contains the higher power $\sin^2(\tau\pi)$ as compared to the $\sin(\tau\pi)$ of the first case in (3.9).

Proceeding as in the previous case,

$$h^{(k)}(\tau) = O\left((\sin(\pi\tau))^{3+\delta-k}\right), \qquad k = 1, \ldots, 4 \tag{3.19}$$

$$H^{(\ell)}(\tau) = O\left([\sin(\tau\pi)]^{\min[\delta/2-\ell+2,0]}\right), \qquad \ell = 0, 1, 2, 3, 4$$

showing $H^{(3)}(\tau)$ and $H^{(4)}(\tau)$ are singular at $\tau = 0$. The second condition stated above, that $\psi_0, \psi_1 \in C^3$ in some neighborhoods of $\tau = 0$ and $\tau = 1$, respectively, is satisfied. Simply use the same approach as in the first case, noting now that in (3.15) the term $\sin(\tau\pi)$ is replaced by $\sin^2(\tau\pi)$. Because of this, all terms arising from (3.16) will be continuous at $\tau = 0$ and $\tau = 1$.

What remains is to show that $\psi_0^{(4)} \in L^1(0, 1)$. Returning to (3.15) for the case $\ell = 4$, the corresponding values of α are

$$\begin{gathered}(4,0,0), (3,1,0), (3,0,1), (2,2,0), (2,1,1), \\ (2,0,2), (1,3,0), (1,2,1), (1,1,2), (1,0,3), \\ (0,4,0), (0,3,1), (0,2,2), (0,1,3), (0,0,4)\end{gathered}$$

Only when we look at terms containing $h^{(4)}(\tau)$ $[\alpha = (0,4,0)]$ or $H^{(\ell)}(\tau)$, $\ell = 3, 4$ $[\alpha = (1,0,3), (0,1,3), (0,0,4)]$, is there any need to check for integrability. It is easily checked that in these cases the corresponding terms in (3.15) are integrable. Thus $\psi_0^{(4)} \in L^1$ in a neighborhood of $\tau = 0$. An analogous result holds for ψ_1 about $\tau = 1$. This completes the proof of Theorem 2.2.

How do we generalize this theorem to larger non-integral values of q? We would again look at two cases:

$$k < q < k + \tfrac{1}{2} \quad \text{and} \quad k + \tfrac{1}{2} < q < k + 1$$

for some integer k. Then we would generalize the formulas for $h^{(k)}$ and $H^{(\ell)}$. The formula for $H^{(\ell)}$ generalizes easily; but that for the composite function $h^{(k)}$ does not. The latter requires using the Faa di Bruno formula (3.11), and we have not found any general way of handling this. It is straightforward to do particular cases, however, and we have suitably generalized (3.13) and (3.19) for $q \in (2, 3)$ and $(3, 4)$. With these results in hand, we then can examine the Leibniz formula (3.15) and show the needed properties for the functions ψ_0 and ψ_1.

4. Superconvergence with $2q$ an odd integer. In [4] it was observed experimentally that with f sufficiently differentiable and $q = 1.5$,

$$I - \mathcal{T}_n = O(h^6)$$

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There was no precise estimate of the speed of convergence for the cases $q = 2.5$ and $q = 3.5$, although it was clear experimentally that the speed of convergence was very high.

As noted earlier following (2.9), we are considering the trapezoidal error $I - \mathcal{T}_n$ when approximating

$$\int_0^\pi F(\theta)G(\theta)\, d\theta \tag{4.1}$$

$$\begin{aligned} F(\theta) &= \frac{(1-q)\sin^2\theta + q}{(\sin^{2q}\theta + \cos^2\theta)^{3/2}} \sin^{2q-1}\theta \\ G(\theta) &= \int_0^{2\pi} f(\xi,\eta,\zeta)\, d\phi \end{aligned} \tag{4.2}$$

Here, resorting to the well-known Euler-MacLaurin expansion in its standard form (cf. [3], [6]), we explain the reason for such superconvergence for the cases $q = 1.5, 2.5,$ and 3.5. Let $p = 4q$, and assume f is p-times differentiable with all p^{th}-order derivatives of f belonging to $L(U)$. Without loss of generality, we can assume that f is defined on some ε-neighborhood of U, call it U_ε, with f having analogous differentiability properties on U_ε. Then we show

$$I - \mathcal{T}_n = O\left(h^{4q}\right)$$

as stated in (2.8) of Theorem 2.3.

Introduce

$$\begin{aligned} \psi(\theta) &= \frac{\sin^q\theta}{\sqrt{\sin^{2q}\theta + \cos^2\theta}} \\ \nu(\theta) &= \frac{\cos\theta}{\sqrt{\sin^{2q}\theta + \cos^2\theta}} \end{aligned} \tag{4.3}$$

and then write $(\xi,\eta,\zeta) \in U$ (see (2.4)) as

$$(\xi,\eta,\zeta) = (\psi(\theta)\cos\phi, \psi(\theta)\sin\phi, \nu(\theta))$$

Since f is sufficiently differentiable over U_ε, we can expand it in a Taylor series about $(0,0,1)$, corresponding to $\theta = 0$, with the series converging in some neighborhood of $(0,0,1)$. Using a Taylor series of order $N-1$, we can write, roughly speaking,

$$f(\xi,\eta,\zeta) = \sum_{\substack{i,j,k\geq 0 \\ i+j+k<N}}^{N-1} a_{i,j,k}\, \xi^i\, \eta^j\, \zeta^k + \rho_N(\xi,\eta,\zeta) \tag{4.4}$$

with appropriate coefficients $a_{i,j,k}$. The remainder $\rho_N(\xi,\eta,\zeta)$ can be written in a variety of forms, each depending on N^{th}-order derivatives of f. Moreover, all derivatives of ρ_N of order $< N$ equal zero at $(\xi,\eta,\zeta) = (0,0,1)$. Using this expansion, we expand $G(\theta)$ about

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$\theta = 0$,

$$
\begin{aligned}
G(\theta) &= \int_0^{2\pi} \sum_{\substack{i,j,k\geq 0\\ i+j+k<N}}^{N-1} a_{i,j,k}\, \xi^i(\theta,\phi)\, \eta^j(\theta,\phi)\, \zeta^k(\theta,\phi)\, d\phi + R_N(\theta) \\
&= \sum_{\substack{i,j,k\geq 0\\ i+j+k<N}}^{N-1} a_{i,j,k} \int_0^{2\pi} \xi^i(\theta,\phi)\, \eta^j(\theta,\phi)\, \zeta^k(\theta,\phi)\, d\phi + R_N(\theta) \\
&= \sum_{\substack{i,j,k\geq 0\\ i+j+k<N}}^{N-1} a_{i,j,k}\, \psi^{i+j}(\theta)\, \nu^k(\theta) \int_0^{2\pi} \cos^i\phi \sin^j\phi \, d\phi + R_N(\theta)
\end{aligned} \tag{4.5}
$$

The remainder $R_N(\theta)$ depends on the N^{th}-order derivatives of f and can be written in an integrated form,

$$R_N(\theta) = \int_0^{2\pi} \rho_N(\xi,\eta,\zeta)\, d\phi$$

Thus $R_N(\theta)$ is well-defined around $\theta = 0$ when the N^{th}-order derivatives of f belong to $L^1(U_\varepsilon)$. In addition all derivatives of $R_N(\theta)$ of order $< N$ equal zero at $\theta = 0$.

Denoting by β the "*Beta function*" (cf. [1, p. 258]), we note that

$$\int_0^{\pi/2} \sin^i\phi \cos^j\phi \, d\phi = \frac{1}{2}\beta\left(\tfrac{1}{2}(i+1), \tfrac{1}{2}(j+1)\right)$$

When i, j are both even, we have

$$\int_0^{2\pi} \sin^i\phi \cos^j\phi \, d\phi = 2\beta\left(\tfrac{1}{2}(i+1), \tfrac{1}{2}(j+1)\right)$$

and this integral equals 0 in all other cases of i, j. As consequence,

$$G(\theta) = \sum_{\substack{i,j,k\geq 0\\ i+j+k<N \\ i,j \text{ even}}}^{N-1} a_{i,j,k}\, \psi^{i+j}(\theta)\, \nu^k(\theta) \int_0^{2\pi} \cos^i\phi \sin^j\phi \, d\phi + R_N(\theta) \tag{4.6}$$

This corresponds to Sidi [11, Lemma 4.1 and Theorem 4.2].

Now let $q = 1.5$. Using *Mathematica* to simplify the calculations,

$$\psi^2(\theta) = \theta^3 + \frac{\theta^5}{2} - \theta^6 + O(\theta^7)$$

$$\nu(\theta) = 1 - \frac{\theta^3}{2} - \frac{\theta^5}{4} + \frac{3\,\theta^6}{8} + O(\theta^7)$$

Use this in the expansion of (4.6), noting that $i + j$ is always even and therefore

$$\psi^{i+j}(\theta) = \left[\psi^2(\theta)\right]^{\frac{1}{2}(i+j)}$$

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with $\frac{1}{2}(i+j)$ an integer. Then

$$G(\theta) = \gamma_1 + \gamma_2\theta^3 + \gamma_3\theta^5 + \gamma_4\theta^6 + O(\theta^7) \tag{4.7}$$

for suitable $\{\gamma_i\}$.

Returning to (4.3), we also have

$$F(\theta) = \frac{3\theta^2}{2} + \frac{5\theta^4}{4} - \frac{9\theta^5}{4} + \frac{77\theta^6}{80} + O(\theta^7) \tag{4.8}$$

Combining (4.7) and (4.8), we have

$$F(\theta)G(\theta) = c_1\theta^2 + c_2\theta^4 + c_3\theta^5 + c_4\theta^6 + O(\theta^7)$$

for suitable constants $\{c_i\}$. A similar Taylor expansion holds for $\theta \approx \pi$. This implies that the first and third derivatives of $F(\theta)G(\theta)$ are zero at $\theta = 0, \pi$.

We apply the Euler-MacLaurin formula to (4.1). Since f is $6-$times differentiable with all 6^{th}-order derivatives in $L(U)$, we can conclude that the order of convergence of the quadrature rule for $q = 1.5$ is 6.

Use an analogous proof when $q = 2.5$ (and assuming f is 10-times differentiable with all 10^{th}-order derivatives in $L(U)$). Then

$$\psi^2(\theta) = \theta^5 + \frac{\theta^7}{6} + \frac{11\,\theta^9}{72} - \theta^{10} + O(\theta^{11})$$

$$\nu(\theta) = 1 - \frac{\theta^5}{2} - \frac{\theta^7}{12} - \frac{11\,\theta^9}{144} + \frac{3\,\theta^{10}}{8} + O(\theta^{11})$$

$$G(\theta) = \gamma_1 + \gamma_2\theta^5 + \gamma_3\theta^7 + \gamma_4\theta^9 + +\gamma_5\theta^{10} + O(\theta^{11})$$

$$F(\theta) = \frac{5\,\theta^4}{2} + \frac{7\,\theta^6}{12} + \frac{11\theta^8}{16} - \frac{15\,\theta^9}{4} + \frac{11077\,\theta^{10}}{30240} + O(\theta^{11})$$

$$F(\theta)G(\theta) = c_1\theta^4 + c_2\theta^6 + c_3\theta^8 + c_4\theta^9 + O(\theta^{10})$$

This allows us to prove that $I - \mathcal{T}_n = O(h^{10})$.

For $q = 3.5$ (assuming that f is $14-$times differentiable with all 14^{th}-order derivatives in $L(U)$)

$$\psi^2(\theta) = \theta^7 - \frac{\theta^9}{6} + \frac{17\,\theta^{11}}{120} + \frac{43\,\theta^{13}}{2160} - \theta^{14} + O(\theta^{15})$$

$$\nu(\theta) = 1 - \frac{1}{2}\theta^7 + \frac{1}{12}\theta^9 - \frac{17}{240}\theta^{11} - \frac{43}{4320}\theta^{13} + \frac{3}{8}\theta^{14} + O\left(\theta^{15}\right)$$

$$G(\theta) = \gamma_1 + \gamma_2\theta^7 + \gamma_3\theta^9 + \gamma_4\theta^{11} + \gamma_5\theta^{13} + \gamma_6\theta^{14} + O(\theta^{15})$$

$$F(\theta) = \frac{7\,\theta^6}{2} - \frac{3\,\theta^8}{4} + \frac{187\,\theta^{10}}{240} + \frac{559\,\theta^{12}}{4320} - \frac{21\theta^{13}}{4} + \frac{9847\,\theta^{14}}{80640} + 2\theta^{15} + O(\theta^{16})$$

$$F(\theta)G(\theta) = c_1\theta^6 + c_2\theta^8 + c_3\theta^{10} + c_4\theta^{12} + c_5\theta^{13} + c_4\theta^{14} + O(\theta^{15})$$

Taken together, this implies that the order of convergence is 14.

We would like to generalize this proof to

$$q = m + \tfrac{1}{2}, \qquad m \geq 1 \text{ an integer}$$

but we have been able to do so for only a portion of it. The difficulty can be seen in the form of the Taylor expansions given above. The various functions are neither even nor odd; but their lower degree terms have the behaviour needed in order to apply the Euler-MacLaurin error formula. Nonetheless what we have shown is sufficient for practical purposes, demonstrating that q of this special form is the preferable choice.

5. Conclusion. Although some of the techniques used in this paper are similar to those used in Sidi [11], they were obtained independently of that paper. A major difficulty with our transformation $\mathcal{L}$ of (2.1) has been the integral term

$$H(\tau) = \int_0^{2\pi} f(\xi, \eta, \zeta)\, d\phi$$

of (3.8). We have had to be quite careful in the handling of its derivatives, as we did in obtaining (3.14) of §3. There is a similar difficulty in Sidi [11, Theorem 4.2], and he has been able to handle it in a different way, by using the general theory he has developed for the error analysis of the trapezoidal rule when applied in connection with class $\mathcal{S}_m$ transformations (cf. [11, Theorem 3.1]). See Sidi [14] for an extension of the results of this paper, completed independently of our present paper. In addition, the papers Sidi [12], [13] also relate to the numerical method studied in this paper, although again our results are obtained independently and are somewhat different in approach.

In spite of the difficulty in the error analysis of our transformation $\mathcal{L}$, we believe it is a natural way to grade nodes on the sphere and one that needs to be understood more fully.

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